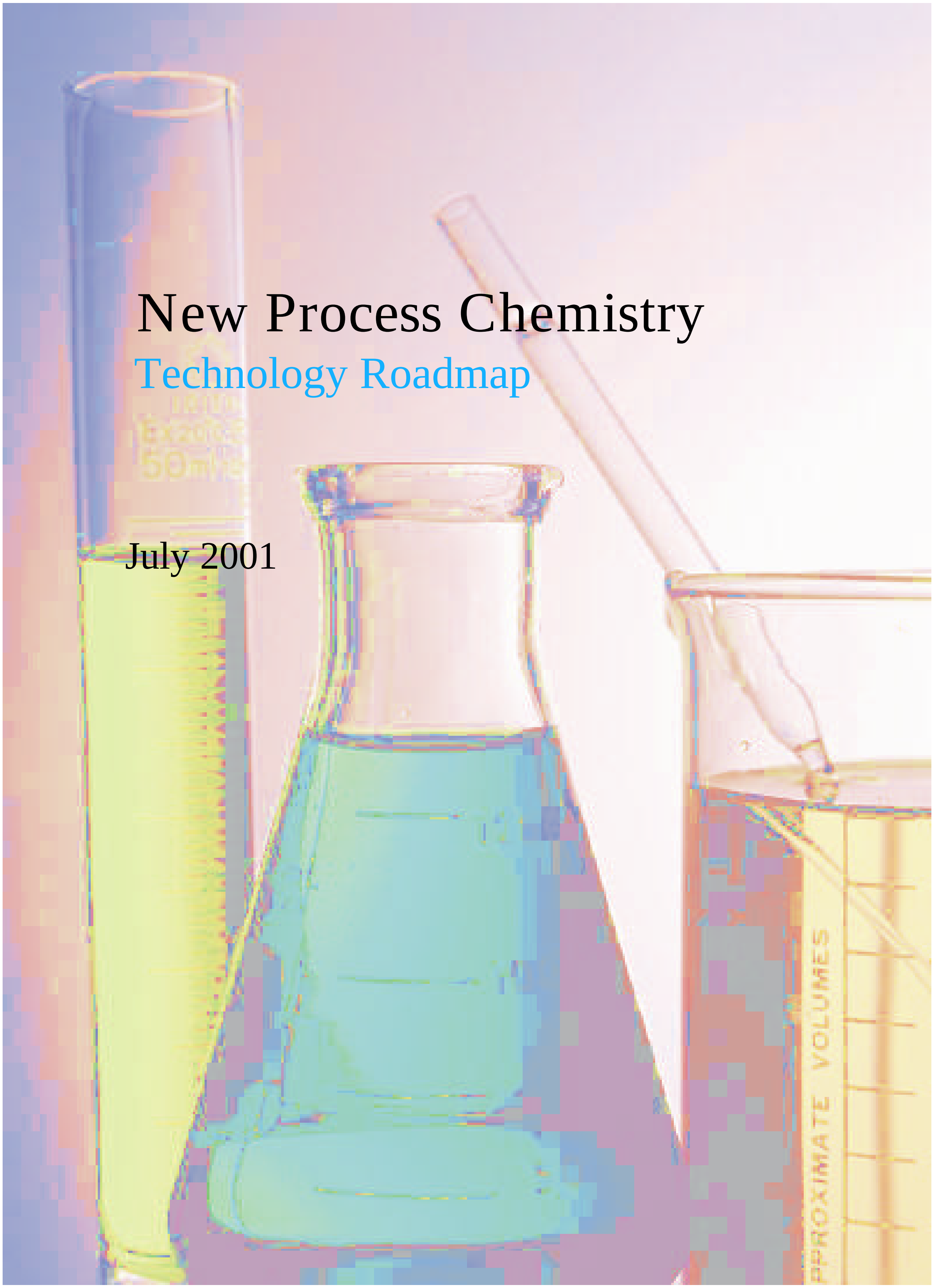
New Process Chemistry

Technology Roadmap

July 2001



Technology Roadmap for New Process Chemistry

Table of Contents

"This roadmap will give us an opportunity to do *way cool* chemistry."

Robert Davidson, 3M, at the *New Process Chemistry Workshop*, Corpus Christi, Texas, February 2000

"It all starts with chemistry."

Joe Zoeller, Eastman Chemical, at the *New Process Chemistry Workshop*, Corpus Christi, Texas, February 2000

"Speaking of the chemical industry and technology partnerships...

...to the extent that companies, government, and universities can get good at this, it is a powerful force for the chemical industry in the 21st century. We can get further faster if we can work together. We haven't had a history of what I'd call close, interdependent partnerships. Companies have pretty much worked on their own and quite frankly it has served us very well for many decades before and after World War II. I think in today's world of globalization, what really hits you square in the face is the need for these partnerships, and we don't have a lot of experience in that."

Richard M. Gross, Corporate Vice President of Research and Development, The Dow Chemical Company, 1998

"We choose to go to the moon. We choose to go to the moon in this decade and do the other things, not only because they are easy, but because they are hard, because that goal will serve to organize and measure the best of our energies and skills, because that challenge is one that we are willing to accept, one we are unwilling to postpone, and one which we intend to win, and the others, too."

President John F. Kennedy, Address to the Nation on the Nation's Space Effort, Rice

Foreword

On June 3, 1996 ACS' *Chemical and Engineering News* carried an editorial entitled "Synergy," by J. Lawrence Wilson, an ACS member and incoming President of the Chemical Manufacturers Association (now called the American Chemistry Council.) In that article, one of several published heralding the release of *Vision 2020* later that year, Mr. Wilson said, "**The world needs more chemistry.** " Our science has brought remarkable progress to society—and created problems along the way. Yet today's chemists also are the key to solving environmental problems. Looking forward, **"the challenge is to discover additional pathways to chemical products and processing which will enhance and sustain the quality of life around the world.**" Reading this again recently we were struck that even back in 1996, Mr. Wilson would have thought it was important for ACS to undertake this *New Process Chemistry Roadmap*.

Fast forward, as the saying goes, to the year 2000 and a sizable number of chemists and engineers who make up the chemical enterprise—industry, academe, and government—have a number of workshops, breakout sessions, conference reports, and draft roadmaps under their belts. Are we. . .

> using *Vision 2020*, as Paul S. Anderson then chair elect of ACS and a Vice President at DuPont Merck said, ". . .as a document that points the way and as a resource to be referred to, worked with and consulted?"
>
> finding, as Mary L. Good, a past ACS President and then Undersecretary for Commerce said, "A lot of useful information in it?"
>
> using *Vision 2020* as Francis A. Via, then Director of Research for Akzo Nobel, said "to orient the R&D activity of government and academe to be more in line with the needs of industry," and
>
> as Mr. Wilson said in his original editorial, "Accomplishing more together than we could separately?"

And have we taken action on the report and gotten value in return as one of us, then Vice President of the PQ Corporation and now Chair of the ACS Board suggested? From what we can see of the far reaching and creative ideas contained in the following pages the answer to this, and all the above questions above, is a resounding, ***yes!*** We can see how taking just one breakthrough idea for new reaction from this chemistry roadmap and applying it again and again to a number of different process chains will create what Mr. Wilson called in 1996 a **synergy** that the entire industry can use to face the energy and environmental challenges ahead. It is our hope that ACS' *New Process Chemistry Roadmap* will inspire all of us to work toward *Vision 2020* common goals that save energy, make the most efficient use of this country's carbon based resources, protect the environment, and ensure the vitality of the chemical enterprise well into the 21st century.

Roger W. Day Chair, Committee on Corporation Associates	Henry F. Whalen Chair of the Board, American Chemical Society	Steven J. Cooke Chair, ACS Industrial & Engineering Chemistry Division

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- Industrial & Engineering Chemistry Division
- Corporation Associates

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Electric Power Research Institute
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- National Environmental Technology for Waste Prevention Institute
- Center for Industry Research on Polymers

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1 Overview

Background

In 1996, over 200 technical and business leaders from the U.S. chemical industry culminated a series of working meetings with the publication of **Technology Vision 2020: The U.S. Chemical Industry**[1]. This report identifies globalized markets, environmental performance, profitability and productivity, customer expectations, and changing workforce requirements as the "five major forces" confronting the industry as it enters the 21st century.

Vision 2020 calls for the industry to set the standard for the efficient use of energy and raw materials and work in seamless partnerships, creating "virtual" laboratories for developing innovative technologies. The study predicts that the next millennium will see a chemical industry that promotes sustainable development by investing in technology that protects the environment and stimulates industrial growth while balancing economic needs and financial constraints. **Vision 2020** concludes that the synergy of collaboration often has a "multiplier effect" on our nation's pool of talent, equipment, and capital available for R&D, and that the chemical industry's growth and competitive advantage *"depends upon individual and collaborative efforts of industry, government, and academe to improve the nation's R&D enterprise."*

Clearly these far-reaching goals for improved productivity, cost-effectiveness, energy use, and environmental performance will require that the industry address both improved, as well as radically new or alternative ways of making chemical products. In support of **Vision 2020** and the pivotal role of new process chemistry, the American Chemical Society (ACS) Division of Industrial and Engineering Chemistry (I&EC) and the Green Chemistry Institute (GCI) jointly sponsored four meetings addressing this topic during 1999. The workshops were attended by participants from industry, government, academia, and the national laboratory complex. Four separate areas of technology were addressed—Dense Phase Fluids and Alternative Reaction Media; the Role of Polymer Research in Green Chemistry and Engineering; Alternative Process Conditions and Electrotechnology; and Synthesis and Processing with Alternative Resources. In February 2000, with the cooperation and support of ACS Corporation Associates, an additional workshop was held to discuss the results of previous efforts, to generate new ideas, and to begin developing a consensus on the technology development needed for innovative new process chemistry[2].

Industrial Chemistry and the Role of Alternative Processes

Where chemistry is the science that deals with the composition, structure, and properties of substances and the transformations that they undergo, industrial chemistry is the practical application and integration of chemistry to the basic science, engineering and marketing that leads to the sale of chemical products.

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[1] Available from the American Chemical Society, Washington, DC, (202) 452-8917.

[2] All five workshops form the basis for this technology roadmap. It is written for a broad audience and the agenda it describes is intended to be used by a wide spectrum of chemists working in high-volume commodity chemicals and specialty chemicals.

Ultimately the goal in using industrial chemistry is to develop a process pathway or a series of reactions that converts relatively abundant, but poorly differentiated raw materials and feedstocks into desirable products for society at the lowest possible cost. Each individual reaction in a process pathway is designed to break the bonds of the **raw material** molecules and ultimately form new molecular bonds for the desired consumer products like paint, plastics, pharmaceuticals, adhesives, fibers, dyes, detergents, and

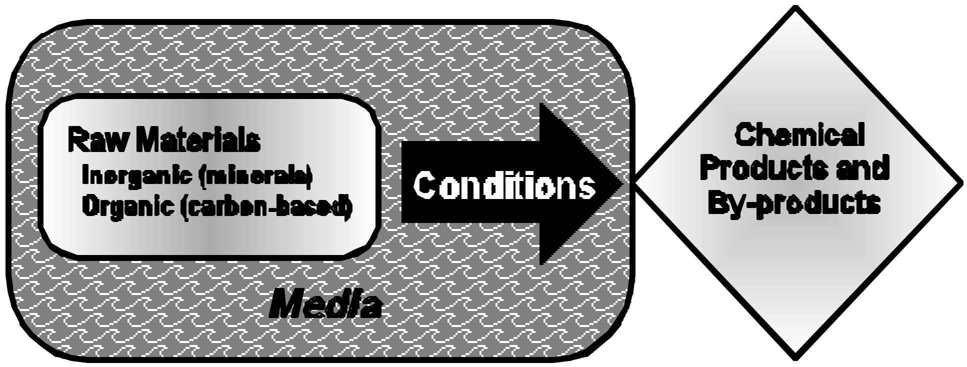


Exhibit 1-1. Chemical Pathways: From Raw Materials to Products

food preservatives. To facilitate these molecular changes a chemist will specify the appropriate **media**, or absence thereof, and the energy-related **conditions** needed to start, continue and stop the reaction (see Exhibit 1-1.)

Exemplary is the petroleum refining industry where the complex groups of molecules that make up crude oil are converted mostly into fuels. Through industrial chemistry, crude oil that is not used for fuels is transformed into petrochemicals—new, highly functional molecules which form the building blocks for more than 70,000 chemical products used by industry and consumers.

Industrial chemists do not accomplish these transformations alone. Engineers are needed to apply engineering principles and analyze each chemical reaction, both individually and in conjunction with all the steps which make up the entire chemical process. The overall objective is to produce chemicals using the raw materials with the lowest cost, minimize capital investment, protect the environment, and ensure the health and safety of those employees that work to manufacture and transport chemical products.

Exhibit 1-2 lists some alternative chemistry and engineering-based technologies, identified during the workshops, that hold the potential to transform the chemical process industry. Alternatives will help to achieve sustainable goals such as reducing units of operation, material usage, waste, and energy use; employing more plentiful or renewable resources; and remaining economically competitive. However, substituting an alternative from the list of traditionally used reaction media, conditions or raw materials may create the need to make further adaptations or changes elsewhere in the process. When all parameters are considered, a lot of work may be needed to radically change a chemical process.

A recent example of how changing one reaction can cascade through the entire process pathway is the development of a new synthetic route for the production of ibuprofen. Changes made from the old process include the introduction of a more selective catalyst, novel reactors that combine an extractor and a distillation column, and the elimination of solvents. The new process, a model of source reduction and winner of a 1997 Presidential Green Chemistry Challenge Award, has only three catalytic steps and approximately 80% atom utilization (virtually 99% when the recovered byproduct acetic acid is considered)[3]. In addition, the new process replaces an inefficient process with six stoichiometric steps, less than 40% atom utilization and company officials estimate saves from 20% to 40% of the total amount of energy when compared to the more traditional process of manufacturing ibuprofen. All starting materials are either converted to products, recovered as byproducts, or completely recycled, virtually eliminating the production of waste.

Exhibit 1-2. Examples of Alternative Technologies

Alternative Media	Alternative Physical Reaction Conditions	Reactions at Interfaces	Synthesis & Processing with Alternative Resources
! Ionic Liquids ! Liquid Polymers ! Aqueous Systems ! High Pressure and Supercritical CO_2 ! Melt Systems (with or without added CO_2) ! Organic Liquids	! Microwaves ! Electrochemical ! Radio Frequency ! Ultrasonics ! Plasma ! Radiation ! Electrical Induction ! Photochemical ! Solar ! Self-assembly ! Catalysts with High Selectivity ! Solvent Elimination	! Solid - Solid (solvent-less) ! Vapor - Solid (including CO_2) ! Solid - Liquid (including CO_2) ! Covalently Attached Thin Liquid Films ! Solvent-free Coatings ! Emulsion ! Suspension	! Alternative Resources (Biomass, Commodity Residues, Natural Gas, Atmospheric CO_2) ! Biosynthetic Pathways ! Biopolymers ! Biomimetic Synthetic Materials ! Biopharmaceuticals

The new ibuprofen process represents an innovation in environmentally sound, efficient technology that has revolutionized manufacturing of bulk pharmaceuticals. The nearly complete atom utilization achieved by the process constitutes a breakthrough in waste minimization, energy efficiency, and cost-effectiveness. Not only can this *New Process Chemistry* approach be used again in batch manufacture but it could also be applied where feasible in continuous manufacture of commodity chemical products.

A Practical Example: New Ibuprofen Process Chemistry

- Processing steps for manufacturing ibuprofen reduced from six non-catalytic steps to three catalytic steps
- Reduces energy consumption by 20-40%
- Virtually eliminates waste
- Winner of 1993 Kirkpatrick Chemical Engineering Award, and the 1997 Presidential Green Chemistry Challenge Award
- Now in use at the BASF plant in Bishop, Texas

[3] "Green Successes," Today's Chemist at Work, February 1999, p.56.

2 The Chemical Industry

Overview of Chemical Industry Products

The chemical industry is a keystone of the U.S. economy, converting raw materials (oil, natural gas, air, water, metals, minerals) into more than 70,000 different products. Few goods are manufactured without some input from the chemical industry. Chemicals are used to make a wide variety of consumer goods, as well as thousands of products that are essential inputs to agriculture, manufacturing, construction, and service industries. About 26% of the total number of chemicals produced are transferred as intermediates (sometimes referred to as performance-based chemical products) used in other chemical processes to make chemicals or products used directly by consumers.

Globally the chemical industry is a $1.5 trillion enterprise, with the industry in the U.S. being the world's largest producer. There are 170 chemical companies with more than 2,800 facilities abroad and 1,700 foreign subsidiaries or affiliates operating in the United States. The industry records large trade surpluses and employs more than a million people in the United States alone[4].

Chemicals are generally classified as **organic** , which are compounds containing carbon-carbon and/or carbon-hydrogen molecular bonds, and **inorganic**, which are compounds that contain elements other than carbon. The industry is divided along similarly, although many chemical companies manufacture both organic and inorganic chemicals. Exhibit 2-1 provides a small sample of chemicals in each category. Interestingly, the manufacture of many chemical products requires the use of both organic and inorganic chemicals (e.g., adhesives, coatings, soaps and detergents).

Exhibit 2-1. Major Chemical Segments

Organic Chemicals	Inorganic Chemicals
• Methane/Methanol	• Industrial Gases (oxygen, nitrogen, carbon dioxide)
• Olefins/Ethylene, propylene	• Ammonia
• BTX (benzene, toluene, xylene)	• Calcium dihydrogen phosphate (agricultural fertilizers)
• Butadiene	• Calcium Carbonate
• Polyols	• Sulfuric Acid
• Phenol	• Phosphoric Acid
• Caprolactam	• Nitric Acid
• Acetone	• Hydrochloric Acid
• Polyethylene	• Chlorine/Sodium Hydroxide
• Polypropylene	• Sodium Carbonate
• Styrene	• Sodium Silicate
• Polyvinylchloride	• Silicon
• Polyurethane	• Titanium Oxide
• Nylon 6 & 66	• Nickel/Iron
• Acetic Acid	
• Polyesters	

[4] The Business of Chemistry 2000, American Chemistry Council, Washington, DC.

On the following pages simple flowcharts are provided to describe some of the organic and inorganic chemical industries (Exhibits 2-2 and 2-3). These chemical product chains are representative of some of the higher volume chemical segments, and are not intended to be inclusive of the entire industry.

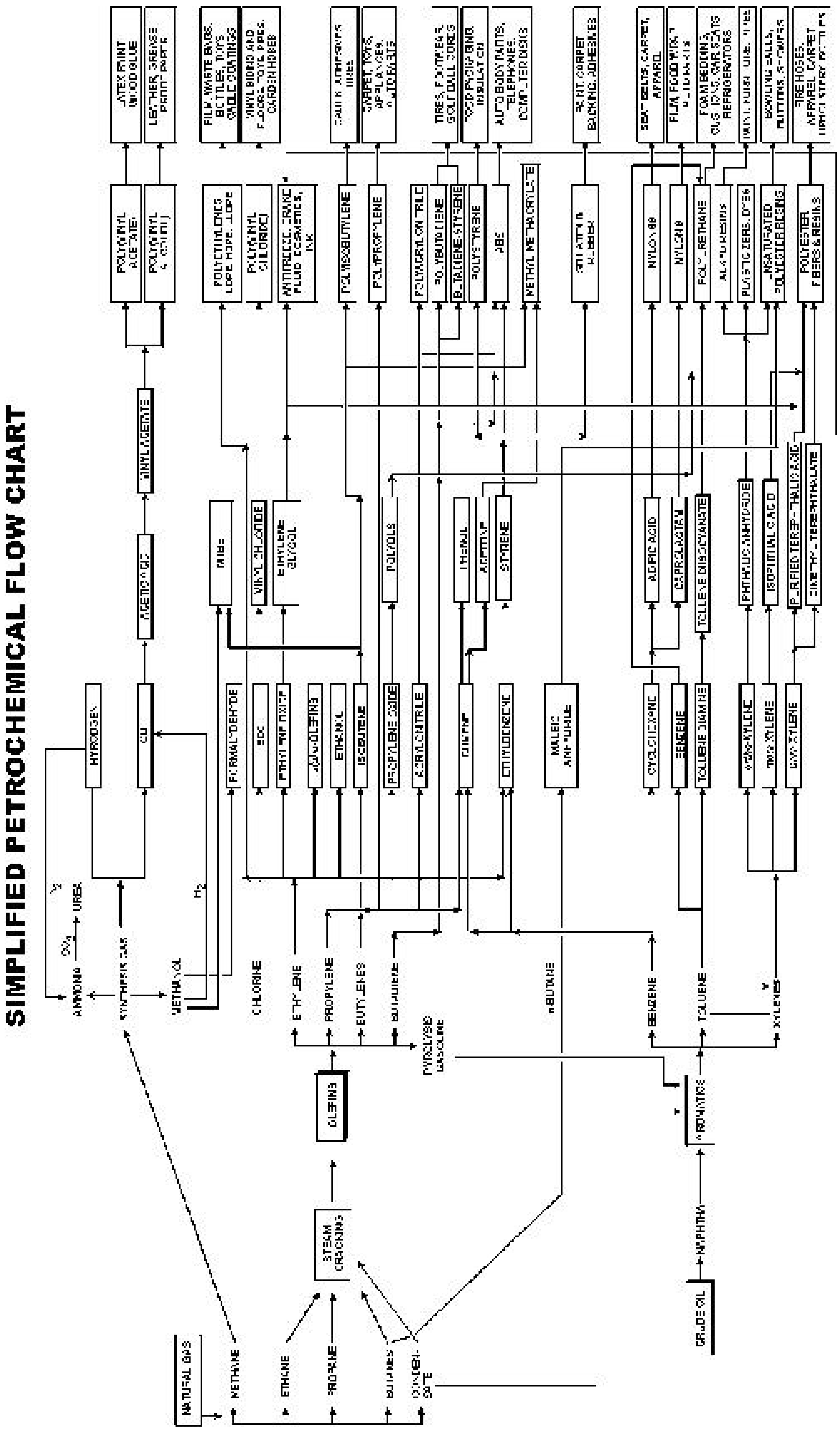
Petroleum, and to a lesser extent, natural gas, are currently the raw materials used for the production of nearly all organic chemicals. Exhibit 2-2 illustrates the chemicals derived from processing of petroleum. One of the important challenges described in **Vision 2020** is to broaden the use of non-petroleum resources (e.g., renewable resources like biomass) in the future as viable substitute feedstock for organic chemicals. The petrochemical industry provides important bulk organic chemicals as well as feedstocks for solvents, plastics, fine chemicals, pharmaceuticals, detergents, soaps, paints, adhesives, and many other chemical products. Ethylene and propylene account for the highest volume of production of petrochemicals (nearly 80 billion pounds annually).

In terms of volume, industrial gases (oxygen and nitrogen), sulfuric acid, ammonia, and chlorine and sodium hydroxide (these are co-produced) are among the top inorganic chemicals produced in the U.S. Although ammonia is made from natural gas (an organic feedstock) ammonia is normally grouped with inorganic chemicals because nearly 90 percent of it is used to produce inorganic chemicals. Inorganic compounds are important inputs to the production of many petrochemicals, plastics, agricultural chemicals (e.g., fertilizers), adhesives, paints, coatings, and soaps and detergents (see Exhibit 2-3).

Common Chemical Processes

The previous discussion and exhibits illustrate the complexity of the chemical industry and the wide array of products. Despite this diversity, there are many common chemistries among the processes and synthetic pathways used in manufacturing chemicals. In some cases the same form of chemical reaction may be used (e.g., oxidation) but under very different reaction conditions. For example, ethylene oxide is made by direct *oxidation* of ethylene over a metal catalyst; phenol is made by *oxidation* with air, followed by acid-catalyzed rearrangement. The central reaction common to both processes is *oxidation*. In fact the new industrial process for making ibuprofen discussed previously decreases the entire chemical pathway from 6 to 3 individual reaction steps - an acetylation, a hydrogenation, and a carbonylation. Although not intended to be an exhaustive list, Exhibit 2-4 illustrates some of the most commonly used chemical reactions.

Exhibit 2-2. Organic Chemicals



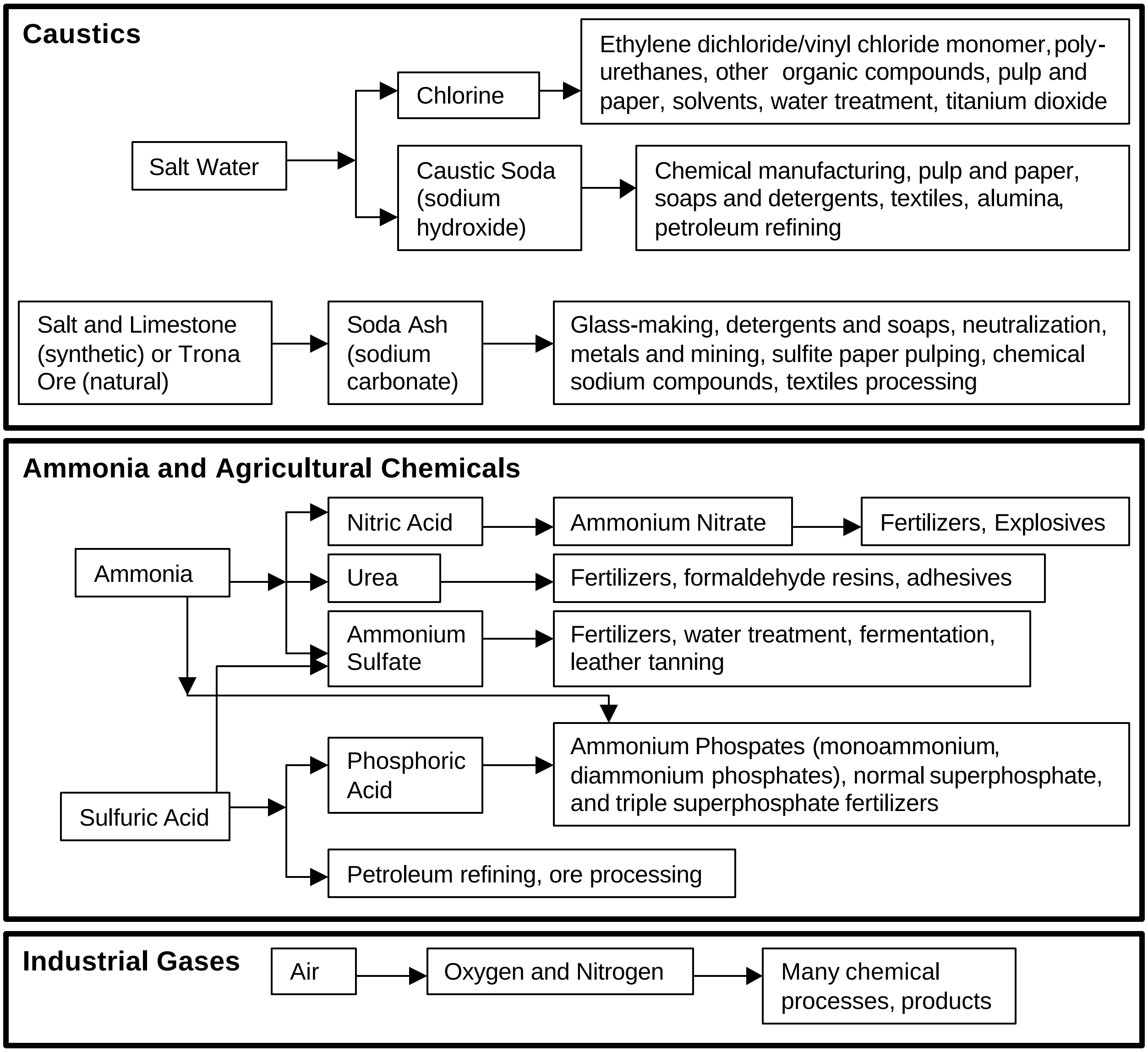


Exhibit 2-3. Inorganic Chemicals

Exhibit 2-4. Chemistry Common to Many Processes		
Type	**Description**	**Exemplary Chemical Product(s)**
Reactions for Organic Chemicals		
Oxidation/ Dehydrogenation (includes epoxidation)	Reaction to increase oxygen content or decrease hydrogen content of an organic molecule	Ethylene oxide, propylene oxide, vinyl chloride, vinyl acetate, acrylonitrile, formaldehyde, isopropyl alcohol, phenol/acetone, styrene, nitric acid, terephthalic acid
Reduction/ Hydrogenation	Reaction to decrease oxygen content or increase hydrogen content of an organic molecule	Cyclohexane
Hydrolysis	Reaction of a substance with water to decompose the original reactant or produce other products; also a reaction of salt with water to create an acid or base.	Ethylene glycol
Chlorination	Reaction to insert a chlorine atom into a chemical compound	Ethylene dichloride, vinyl chloride
Carbonylation	Reaction to introduce carbon monoxide into a molecule or species to create a carbonyl	Aldehydes and ketones, acetic acid
Acetylation	Reaction to introduce an acetyl group (CH_3CO-) into an organic molecule with -OH or -NH_2 groups	Acetic anhydride, acetyl chloride, aspirin, Tylenol™
Polymerization (addition, solution, suspension)	Combination of two or more monomers or alkenes (C=C) to form polymers; can be liquid or gas phase, catalytic or non-catalytic.	Polyolefins (polyethylene, polypropylene), polystyrene
Polymerization (condensation)	Combination of two or more monomers at each step, with condensation of a byproduct.	Polyamides, polyesters
Alkylation	Reaction of an alkane (C-C) with an alkene (C=C), usually in the presence of an acid.	Ethylbenzene, cumene
Electrolysis	Electrochemical reaction using an electrolytic cell to produce chemical products.	Hexamethylenediamine, adiponitrile
Reactions for Inorganic Chemicals		
Electrolysis (high voltage)	Reaction of silicon oxide (SiO_2) with carbon to produce silicon carbide (SiC) and finally Si.	Elemental silicon
Polymerization (condensation)	Direct conversion of silicon to dimethyldichlorosilane, which then polymerizes through a series of hydrolysis-condensation processes.	Silicones
Electrolysis	Electrochemical reaction where sodium chloride (NaCl) in a brine solution separates electrolytically into sodium hydroxide and chlorine.	Chlorine, sodium hydroxide
Separations		
Distillation	Separation of a liquid mixture by boiling points in a column filled with sieve trays or packings	Nearly all organic chemicals
Crystallization	Formation of solid particles within a homogeneous phase; crystallization from liquid solution is most industrially important.	Terephthalic acid, isomers of xylene, agricultural chemicals, inorganic chemicals.
Steam Cracking/Steam Reforming	Pyrolysis of hydrocarbons in the presence of steam	Ethylene, propylene, benzene, toluene, xylene, ammonia

3 Performance Goals

For this roadmap to support **Vision 2020** and assist the industry in making progress toward the broader strategy described in Chapter 1, workshop participants and roadmap contributors developed a set of performance-based goals. Performance goals are an important part of any strategy, as quantitative targets enable research managers and corporate decision-makers to evaluate progress. In general, these goals focus efforts on using energy and material resources more efficiently, reducing emissions and waste streams, improving the productivity and profitability of the chemical industry, and increasing a scientist's access to the enabling tools needed to support successful and productive R&D (see Exhibit 3-1).

Exhibit 3-1. Overall Performance Goals for 2020

- Reduce feedstock losses to waste and byproducts by 90%
- Reduce energy intensity by 30%
- Reduce emissions, including CO_2 and effluents by 30%
- Increase use of C1 compounds by 20%, and use of renewables by 13%
- Reduce the time to market through the use of new R&D tools by 30%
- Increase the number of new products and applications annually by 15%
- Reduce production costs by 25%

Achieving a sustainable chemical industry by 2020 and reducing what some call "planetary stresses" will require a reduction in the use of both energy and raw materials. The goals shown in Exhibit 3-1 to reduce the (1) proportion of feedstock that ends up as waste, (2) low value byproducts, (3) emissions and effluents, and (4) energy intensity of an industrial process are all grounded in theories of *atom economy or source reduction* as well as engineering analyses to determine the process *mass and material balance* . Ultimately the R&D performed and the technology developed as a result of the **New Process Chemistry Roadmap** will enable the industry to reach these goals by minimizing the amount of carbon-based materials going into waste streams, decreasing the severity of operating conditions (temperature and pressure), reducing equipment and facility corrosion and wear, minimizing shutdowns and downtime, and putting more selective catalysts to work achieving larger yields or more product and less by-products with the same amount of energy.

The performance goals corresponding to a reduction in time to market, an increase in the number of new products and applications, and a reduction in production costs as shown in Exhibit 3-1 will result from new R&D and design tools like computational modeling, combinatorial techniques, and from studies in reaction engineering. These goals will be achieved by enhancing energy and material efficiencies, using inexpensive renewables like plants, crops, or woody materials, industrial wastes or byproducts, and even novel alternative materials like the C1 compounds carbon monoxide, methane, and where appropriate carbon dioxide.

4 R&D Opportunities

The next step in charting the course for *New Process Chemistry* is to identify and prioritize R&D opportunities (see Exhibit 4-1.) Characteristics that would be essential to attain for each R&D area of process chemistry, and how each relates to overall performance goals are illustrated in Exhibits 4-2 to 4-6. Each exhibit also includes links to the engineering areas that are supported by research in new process chemistry.

Exhibit 4-1. R&D Needs for New Process Chemistry

Priority	Novel Feedstocks	Reaction Media	Process Conditions/Equipment	Cross Cutting
HIGH	New/better technologies (from catalysts to reactors) for conversion of C1 molecules (e.g., photocatalysts, thermal catalysts, electrocatalysts, low temperature conversion) Cost-effective production and selective catalytic-methods for use of H_2O_2, N_2 and O_2 Catalysts for photo-decomposition of water into hydrogen, and photochemical CO_2 fixation Capability to use formate esters and other CO_2-derived molecules as chemical building blocks	Exploration of entirely new chemistries in new media Solvent-less processes for polymerization and organic chemicals Differentiated examples of key chemistry with improved yield and selectivity (base or acid-catalyzed, reduction-oxidation) Alternative processing media (e.g., supercritical media, water, plasmas) Kinetics and thermodynamics of mass transport processes in alternative media (time limits, polar/non-polar solvents, surfactant behavior, diffusion coefficients, viscosity, dissolution rates)	Alternative reactor concepts (biomass & petrochemical) New cells/cell chemistry for chlor-alkali production Novel, scalable reactor designs using alternative techniques such as plasmas, microwaves, electrochemistry, photochemistry Lower cost/better performance materials for electrochemical processes	New catalysts for carbon/carbon, carbon /hydrogen and carbon/nitrogen bond activation Improved catalytic selectivity Chemistry at interfaces and in multi-phase systems Catalysts to polymerize lower-purity monomers Mechanistic understanding of enzymatic catalysis for polymer production Metabolic engineering to control structure and features of polymers Electrocatalysis (role of acceptors, mechanisms of degradation)

Exhibit 4-1. R&D Needs for New Process Chemistry

Priority	Novel Feedstocks	Reaction Media	Process Conditions & Equipment	Cross-Cutting R&D
MEDIUM	Improved methods for generations of synthesis gas (e.g. any carbon-based gas) New applications and processes for CO_2 (where free energy such as solar is used to transfer energy to CO_2 for activation) Catalytic processes (catalyst and reactor design for chemical synergy from C2 molecules) Short contact time conversion processes for methane	Interfacial science (surface design, nucleation, stability of colloids, interfacial tension, emulsions, fibers, thin films) Use of near-critical H_2O for organic synthesis Low-emission, continuous processing technology for polymerization in alternative media Physical and chemical properties data for new reaction systems Development and testing of dense phase fluid equipment capable of handling material and debris (pumps, compressors, valves, heat exchangers) Solubility database for existing and new solvents	Continuous processing systems (e.g., bulk solids, large dimension products, using electrotechnology) Catalysts for photochemical reactions Hybrid separation techniques that combine a biological step Improved novel bioreactors Better tools to exploit non-steady state reaction processes *In situ* methods for generating high energy compounds as intermediates Non-conventional heating and cooling techniques (e.g. microwaves, liquid nitrogen)	Media/techniques for improved selectivity of chiral versus achiral products Combinatorial techniques applied to catalysts and enzymes for polymer design High through-put methods for catalyst synthesis and testing Better understanding of structural requirements for biodegradability of polymers Fundamental processes controlling self-assembly Depolymerization mechanisms Selective catalytic oxidation of organic matter using oxygen Catalysts for conversion of solar to chemical energy (non-nuclear)

Priority R&D Opportunities

Novel Feedstocks—There are a number of areas where new feedstocks can improve atom economy and resource efficiency by minimizing waste and byproducts. Using C1 compounds, or one-carbon compounds, are an important area for feedstock development. Selective processes are needed to convert C1 compounds into high-value derivatives (C5 and greater), including new catalysts as well as reactor designs. One suggestion is to take advantage of plant photosynthesis reactions, where CO_2 is converted into a carbohydrate by the free energy of the sun. Another idea is to explore how energy, in the form of light, can be used as a gathering system to transfer energy to CO_2 for activation, and then continue to react with the next feedstock in the process.

Reaction Media—More needs to be known about the physical and chemical characteristics of different materials before they can be used as reaction media. Data characterizing the thermodynamic, solubility and toxic properties of these potential media would support modeling that could contribute to predicting reaction behavior and kinetics. In addition, new processes based on new media would eventually require new equipment and reactor designs, new separation techniques, and new heat transfer data. Ideas for new media include solvent-less reaction environments and non-hydrocarbon solvents like ionic liquids, aqueous or melt systems, and dense phase gases. For this area a key R&D opportunity is to develop new chemistry using new media and in turn improve the industry's cost effectiveness through the life cycle of the process.

Process Conditions and Equipment—New process chemistry discussions explored the need for advanced reactor concepts like novel reactors that incorporate a catalytic system, sonic reactors, micro-reactors, short-contact time reactors, and innovative designs using membranes either alone or in hybrid configurations. Key performance characteristics for new reaction conditions will require lower costs (capital, materials, downstream processing), more uniform reactions, increased processing flexibility and even a reduction of carbon dioxide in particular when generated as a byproduct during oxidation processes. Reduction of carbon dioxide will become increasingly important as industry attempts to limit the amount of carbon dioxide it emits. This might be accomplished through improvement in catalyst selectivity or changes in processing conditions. Another important research area is the development of new cells and cell chemistries for chlor-alkali production (chlorine and sodium hydroxide, which are co-produced in an electrolytic cell). Chlor-alkali cells are large consumers of electricity, and there are significant opportunities to improve cell efficiency. A performance target was identified for reducing cell energy requirements by 30%.

Cross-cutting R&D—Some R&D opportunities can be classified as cross-cutting, i.e., they will support development of new process chemistry in several areas (media, conditions, feedstocks). Catalysis is a key example of cross-cutting research, and a high priority research area. The highest priority R&D in this area is the development of new catalysts for carbon/carbon and carbon/hydrogen bond activation, particularly oxidation catalysts. These catalysts will be essential for further development of C1 compounds as feedstocks, as well as new media. The development of catalysts with improved selectivity is another high priority R&D opportunity. Key areas of R&D include enantio-selective catalysts, and selective catalysts for production of some important chemicals (e.g., olefin epoxide, selective alpha olefins, and others). Another potential area for improving selectivity is through the use of external energy inputs such as plasmas and microwaves.

Exhibit 4-2. New Reaction Media

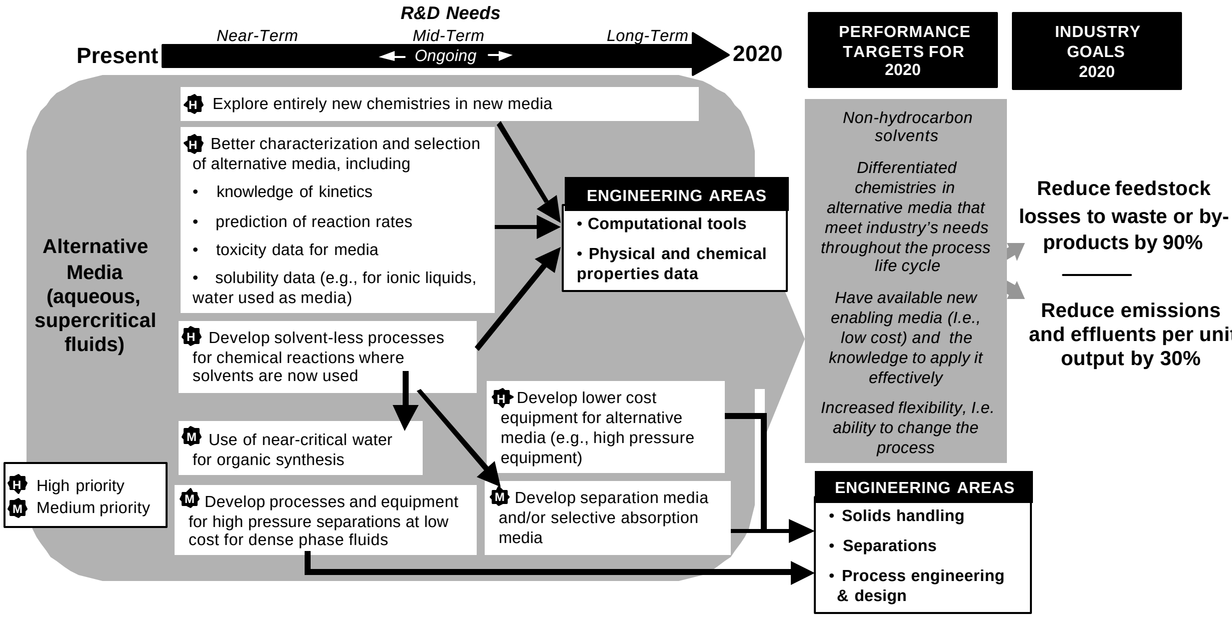


Exhibit 4-3. Catalysis and Other Cross-cutting R&D

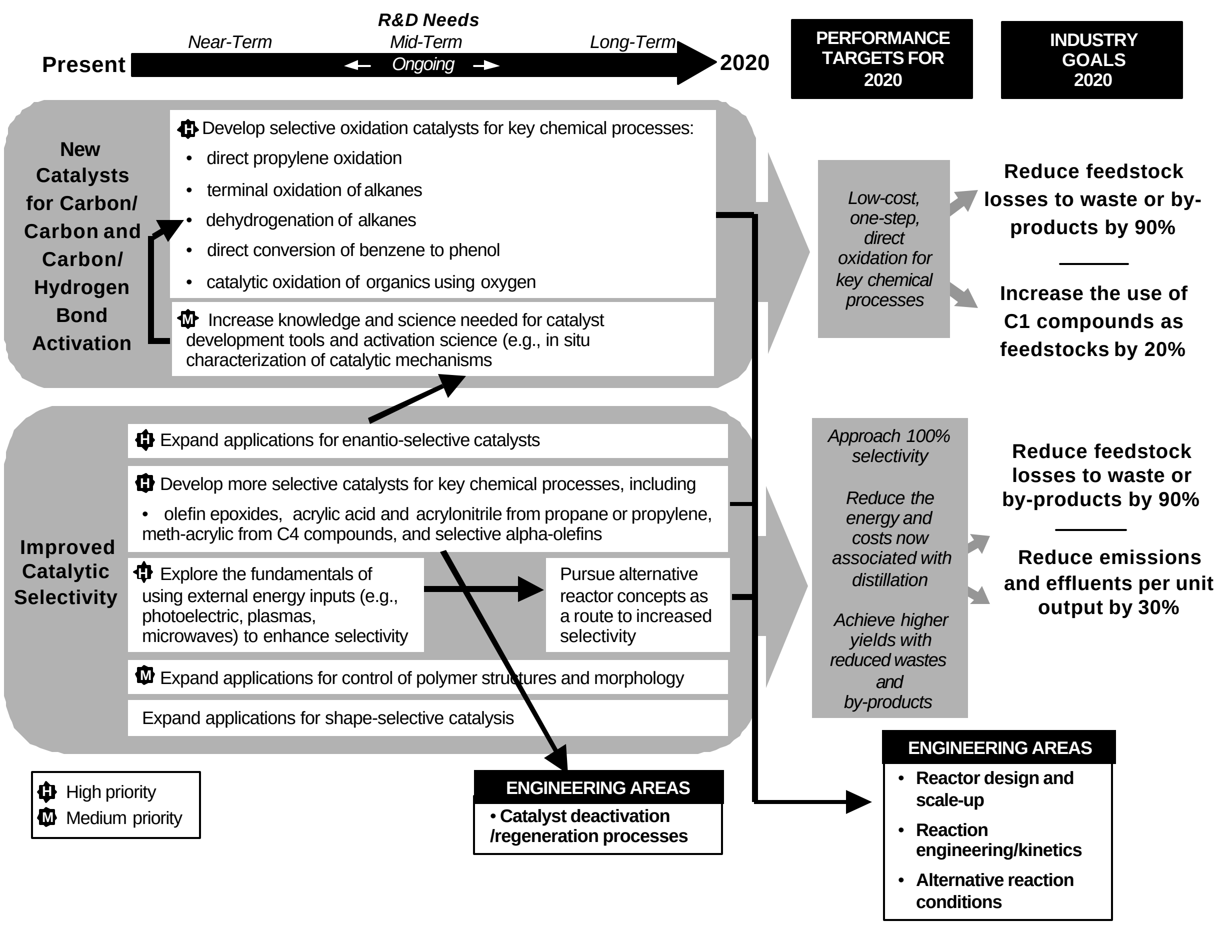


Exhibit 4-4. Catalysis and Other Cross-cutting R&D

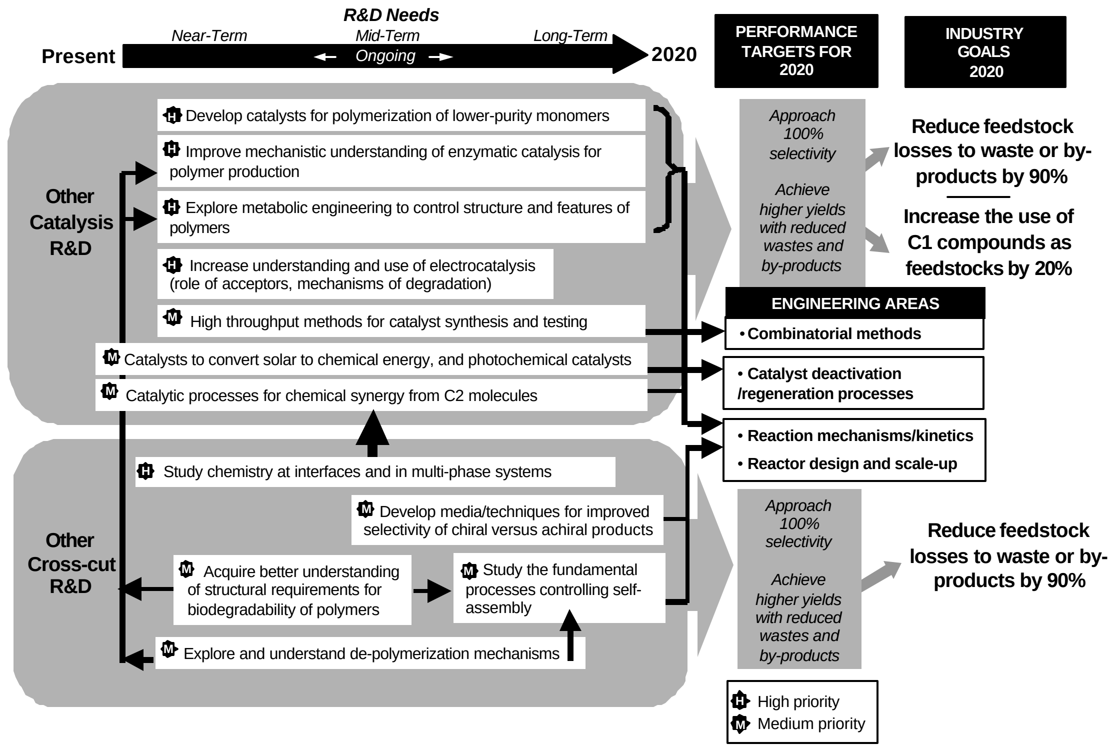


Exhibit 4-5. Process Conditions and Equipment

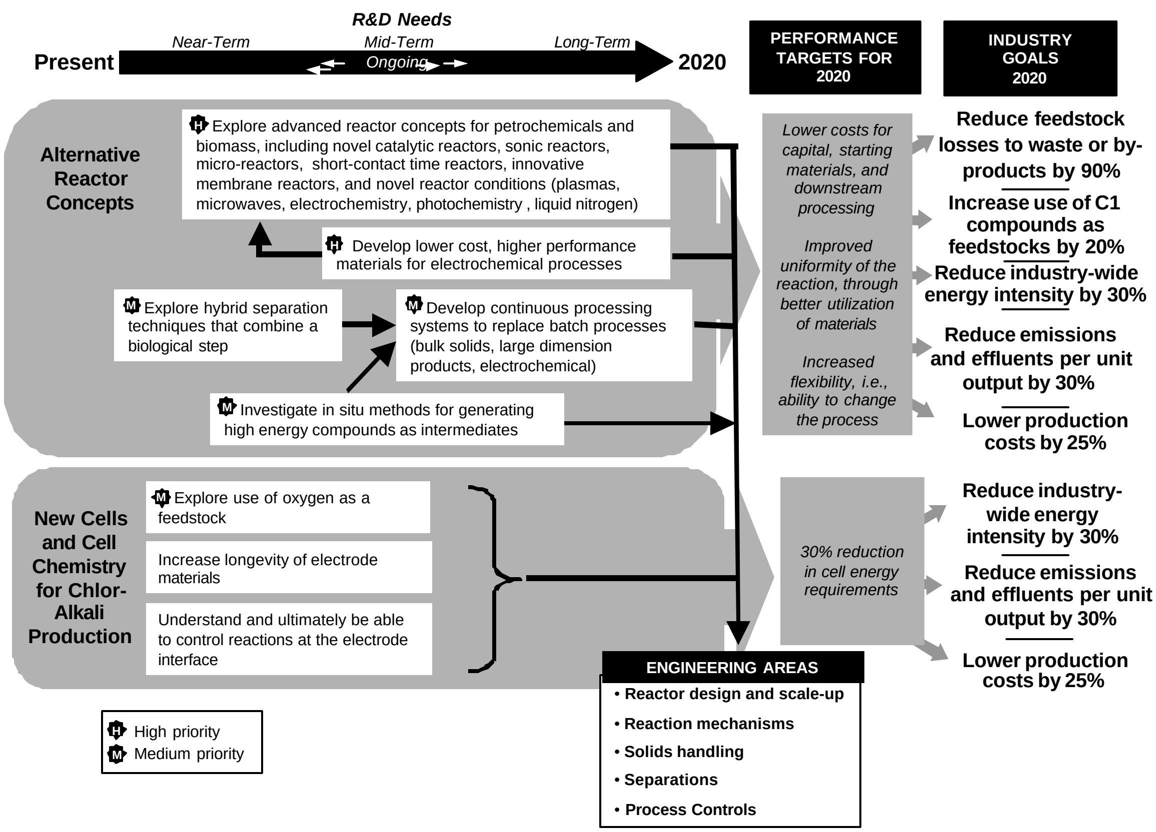
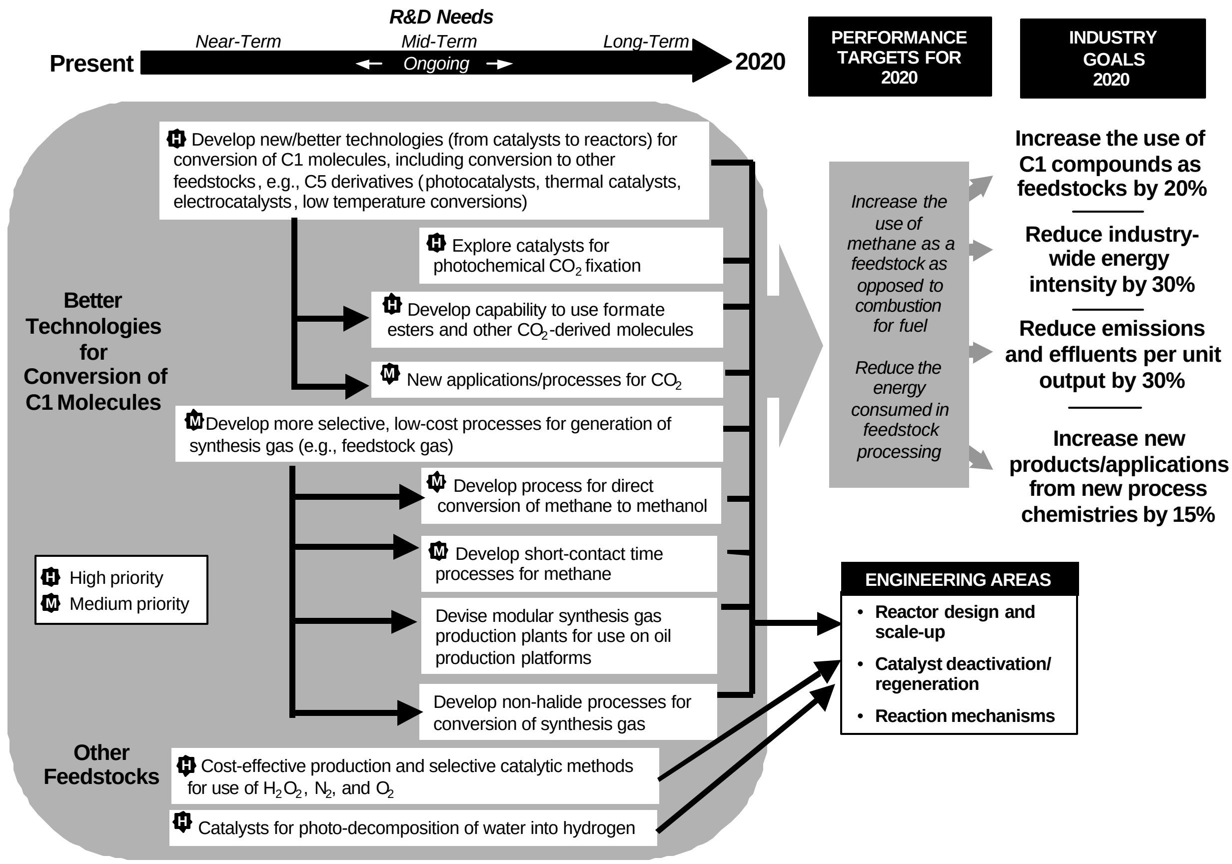


Exhibit 4-6. Novel Feedstocks



Enabling R&D Tools

Enabling research tools are needed to improve the productivity of the R&D process and reduce the amount of time it takes to transform research into viable new processes and products. Enabling tools can provide researchers with the data and computational methods needed to analyze and compare the performance of new process chemistries. Exhibit 4-7 illustrates the R&D needed to improve R&D productivity. Accurate models for early economic screening of new process chemistries were identified as a high priority.

Combinatorial techniques could also prove to be a very important part of the screening and development pathway for catalysts, media, and new process options. Other high priority areas are better tools for catalyst design, and predictive capability for the performance and properties of polymers based solely on molecular structure.

Exhibit 4-8 describes some of the specific R&D topics within the two highest priority areas. Early screening approximate models are a priority R&D need for models used for economic and feasibility screening. In the area of combinatorial techniques, a high priority is the development of single-site architecture in heterogeneous catalysts.

Exhibit 4-7. R&D for Development of Enabling R&D Tools

(✪ = Top Priority; **M** = High Priority; **F** = Medium Priority)

Develop models to provide early economic and feasibility screening for process options
✪✪✪M F F

Apply combinatorial techniques to catalyst development in a general way
✪✪✪MMM F

Develop tools to better understand/design catalysts
MMM

Establish optimum model for collaboration among government-industry-academia
✪

Develop ability to predict polymer properties and performance from molecular structure
M

Revisit previous options that were limited for various reasons
M

Improve methods of retro-design
F

Devise methods for small-scale information generation
F

Conduct life-cycle analysis of major polymers with regard to economics and environmental impacts

Exhibit 4-8. R&D for Development of Enabling R&D Tools

Priority	Early Economic Feasibility Screening of Alternatives	Computational Design of Alternatives	Combinatorial Techniques
HIGH	Develop models to provide early economic and feasibility screening for process options including S early screening approximate models S models to explore the chemistry of alternatives early-on in the design process S economic models for process screening	Develop and experimentally validate models covering S statistical mechanics S physics-based methods S un-contained dense phase conditions S complex fluids S quantum mechanics S equations of state Develop reliable tools to better understand and design catalysts Develop integrated models at multiple scales Predict macro-properties of polymers from molecular properties	Develop combinatorial techniques for catalysts, alternative solvents, and process options including S single-site architecture in heterogeneous catalysts S general combinatorial techniques for catalyst development

Exhibit 4-8. R&D for Development of Enabling R&D Tools			
Priority	**Early Economic Feasibility Screening of Alternatives**	**Computational Design of Alternatives**	**Combinatorial Techniques**
MEDIUM	Develop improved methods of life-cycle analysis for new vs existing reactions/processes Conduct life-cycle analysis of major polymers with regard to economics and environmental impacts	Develop ability to predict polymer properties and performance from molecular structure Improve methods of retro-design Devise methods for small-scale information generation	Combinatorial techniques applied to catalysts and enzymes for polymer design

Other R&D Topics

Additional R&D opportunities were identified in other chemical industry roadmaps (see Exhibit 4-9). These were not discussed at length in this report, but are considered overall as important research areas. For additional information on these topics, refer to the indicated roadmaps (availability information is provided in Chapter 5).

Exhibit 4-9. R&D Topics Addressed in Other Roadmaps	
R&D Topics	**Roadmap(s)**
Metabolic/enzymatic pathways for large-scale chemicals production Metabolic engineering to design and add value to plants and biomass used as chemical feedstocks Polymer synthesis from natural sources (bio-derived monomers) New processes and chemistry for biomass feedstocks Separation and purification of biofeedstocks Naturally-derived biobased polymers	Materials Technology, Biocatalysis, Renewable Bioproducts, Separations/Dilute Solutions
Better separation technology, including low-cost alternatives to distillation	Separations

5 The Road Ahead

On the page facing the Foreword at the beginning of this report are insightful quotes from Richard M. Gross, an industry advocate of Vision 2020 partnerships, and from President John F. Kennedy on the Nation's space effort in 1962. Many will remember the enormous devotion and hard work that came together for this country to go the moon. What is particularly striking when hearing that speech again is the concept that *we choose to do this not because it is easy but because it is hard.* For chemists, the challenge those words of motivation must have inspired need no explanation. This is precisely why many choose to become chemists -- because it is hard. It is hard to improve catalytic selectivity and to understand the kinetics and thermodynamics of mass transport. It is hard to reduce feedstock losses to waste and byproducts by 90%. It is hard to reduce the time to market through the use of new R&D tools by 30%. These and other challenges are what inspires chemists to explore and create revolutionary concepts.

Part of why chemistry is hard is that there is no single discipline of science or technology (e.g., catalysis, computational chemistry) that will in and of itself be able to revolutionize an industry as diverse as the chemical industry. In reality, the chemical industry is complex and interdependent, producing a wide variety of products from pharmaceuticals to plastics. This diversity requires an equally wide variety of engineering, chemical, biological, physical science and logistical specialties all working in concert to produce products. To pursue the far-reaching goals of this roadmap might logically demand that the industry be divided into groups that have chemistry and industrial processes in common. However, in practice, the solutions needed to meet the ambitious goals of this roadmap will not be found in the isolation of separate groups.

As the links drawn in the exhibits in Chapter 4 demonstrate, virtually all the research and development needed will require coordination with activities in multiple scientific and technical fields. As scientists we know that it is not sufficient to improve the chemistry of polymerization with a new catalyst without considering other fields of engineering like reactor system design and scale up, fluid mechanics and transport, separations, catalyst deactivation and regeneration, solids processing and process control.

In the spirit of doing real chemistry it is clear that no one roadmap will be sufficient for an industry that is as diverse as the chemical industry. *New Process Chemistry* begins in the laboratory but of necessity reactor design, reaction engineering, feedstock cost and availability, and downstream processes like separations all come into play.

Chemical Industry Roadmaps and Workshops

- Computational Chemistry
- Computational Fluid Dynamics
- Combinatorial Methods
- Separations
- Materials of Construction in the CPI
- Reaction Engineering
- Biocatalysis
- Materials Technology
- Catalysis

Outside of this *New Process Chemistry Roadmap* supported by the American Chemical Society, the chemical industry has been working on developing a number of roadmaps, some of which address these important topics in detail. Readers are encouraged to keep up-to-date on the progress of these roadmaps or to download copies by visiting the Council for Chemical Research web site at www.ccrhq.org. Additional information and links to roadmap sites can be found at the U.S. Department of Energy web site at www.oit.doe.gov. This roadmap and related workshop reports can be found at http://membership.acs.org/i/iec.

Appendix A

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